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Title: MOMENT-BASED EFFECTIVE TRANSPORT EQUATIONS FOR ENERGY STRAGGLING

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Moment-Based Effective Transport Equations for Energy Straggling

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Ion energy straggling is accomodated in condensed history (CH) Monte Carlo simulation by sampling energy-losses at the end of a fixed spatial step from precomputed, pathlength dependent energy-loss distributions. These distributions are essentially solutions to a straight ahead transport equation given by

$$\frac{\partial \psi(s,E)}{\partial s} = \int_{Q_{min}}^{Q_{max}} dQ\, \sigma_e(E,Q)\psi(s,E+Q) - \sigma_e(E)\psi(s,E), \quad s \geq 0, \tag{1}$$

with monoenergetic incidence $\psi(0,E) = \delta(E_0 - E)$. In Eq.(1), s is the pathlength variable, $\sigma_e(E,Q)$ is the differential cross section for energy loss Q, typically given by the relativistic Rutherford cross section for hard collisions [1, 2], $\sigma_e(E)$ is the total ion-electron scattering cross section, and Q_{min} and Q_{max} are, respectively, the minimum and maximum energy transfer per collision. Direct solution of Eq.(1) by stochastic or deterministic numerical techniques is not feasible because of the very small energy transfers and very small mean free paths that characterize charged particle interactions. Condensed history codes typically employ an approximate solution due to Vavilov [1], obtained assuming a constant mean free path and thus restricted to short step sizes. This solution is formal and its numerical evaluation can be computationally laborious, especially for small step sizes. In practice, Monte Carlo codes have incorporated the Vavilov theory through elaborate numerical approximations, such as truncated Edgeworth expansions, curve-fitting approximations using Moyal functions for small penetration depths or higher energies, and special treatments for the large energy-loss tail of the distribution. [3]

In this paper we propose an alternative approach which is also valid under the conditions of the Vavilov theory but has the potential of being computationally more efficient. We begin by expressing Eq.(1) in the following purely local or differential form

$$\frac{\partial \psi(s,E)}{\partial s} = \sum_{n=1}^{\infty} \frac{1}{n!}\frac{\partial^n}{\partial E^n}\left[Q_n(E)\psi(s,E)\right]. \tag{2}$$

where $Q_n(E) = \int_{Q_{min}}^{Q_{max}} dQ Q^n \sigma_e(E,Q)$, $n = 1, 2\cdots$, are energy-loss moments. We note that Q_1 is just the mean energy loss or stopping power (S) while Q_2 is the mean-square energy loss or straggling coefficient (T). Equation (2) shows that the spectrum is completely characterized by these energy-loss moments and that increasingly more accurate physics can be captured by retaining successively higher order energy-loss moments. In particular, truncating the expansion in Eq.(2) at lowest order yields the continuous slowing down approximation which only preserves the first moment or the mean energy loss. Straggling is introduced by also retaining the mean-square energy loss moment Q_2, giving the Fokker-Planck approximation, and this yields a Gaussian energy spectrum which is accurate for thick targets or at low energies. At higher energies or for thin targets, higher moments must be preserved but it can be shown that truncation orders higher than second (i.e., strictly Fokker-Planck) are not stable. For instance, the third order term introduces unphysical oscillations in the sprectrum while retaining the fourth order term yields an unbounded solution. However, the generalized Fokker-Planck expansion reveals the central role played by these energy-loss moments, and furthermore suggests the following moment-based approach to computing straggled spectra for finite step CH simulations: approximate the collision integral such that a finite number of low order energy-loss moments are *exactly* preserved whilst all higher order moments are approximated in terms of these lower order moments. The expectation is that by not preserving all moments rigorously, the resulting energy loss kernel will be less forward peaked, and the mean free path longer, than the actual, leading to a computationally more efficient transport process. Moreover, the approximation is systematic in that preserving more moments yields an increasingly more refined solution. We note that a related approach has recently been used to deal with forward peaked angular scattering [4]. After some analysis, our effective transport model takes the form

$$\frac{\partial\psi(s,E)}{\partial s} = \int_E^{E_0} \sum_{k=1}^{K} \left[\frac{\hat{\sigma}_k}{\beta_k} e^{-(E'-E)/\beta_k}\right] \psi(s,E')dE' - \hat{\sigma}_t \psi(s,E), \tag{3}$$

where $\hat{\sigma}_t = \sum_{k=1}^{K} \hat{\sigma}_k$ is the effective total cross section. The parameters $\{\hat{\sigma}_k,\, \beta_k,\, k = 1, 2\cdots K\}$, are chosen to rigorously reproduce the first $2K$ energy-loss moments of the exact cross section, and we conjecture that in the limit as $K \to \infty$ the approximate model will reproduce the exact model. We have considered this model for $K = 1$ and $K = 2$ specifically. The former case preserves the mean and mean-square moments exactly and yields $\beta_1 = \frac{T}{2S}$, $\hat{\sigma}_1 = \frac{2S^2}{T}$. For $K = 2$ the free parameters are nonlinearly related to the first four moments but accurate explicit approximations can be readily constructed.

We have obtained closed form solutions to Eq.(3) for the two- and four-moment theories in terms of readily computable special functions. These solutions are compared against straggled spectra obtained from (i) analog or single event Monte Carlo simulation of the exact transport process given by Eq.(1), (ii) the Vavilov theory as implemented in the MCNPX code [5, 6], and (iii) a Gaussian solution. Numerical results have been obtained for 1700 MeV protons incident on a tungsten target, with the straggled spectra for 1 and 2 cm slab thickness displayed in Figure 1 and the spectra for 0.5 cm shown in Figure 2. It is clear from these results that the four-moment theory is highly accurate and captures the skewness in the spectra very well. While the two-moment results appear more accurate than the Gaussian, particularly in the tails of the distribution, both are unacceptably inaccurate. Thicknesses in excess of 20 cm are necessary before the lowest two moments dominate the straggling enough for the two-moment solution to be accurate, although the assumptions underlying the Vavilov model may become questionable under these conditions. For thicknesses less than 0.5 cm the four-moment theory is less accurate as the spectrum becomes highly asymmetric with long low energy tails. Nevertheless, the accuracy of the spectrum realized with only four moments is striking. The Vavilov distribution captures the high energy part and the peak of the distribution accurately but displays artefacts in the low energy (large energy-loss) tail. This phenomenon is currently being investigated further. The results of this study clearly show that moment-preserving effective transport models provide a viable alternative to the Vavilov theory for energy loss straggling in thin slabs. An assessment of the computational efficiency of this approach, based on both single event Monte Carlo simulation and direct discretization of the effective transport model given by Eq.(3), as well as several other issues, forms the subject of ongoing work.

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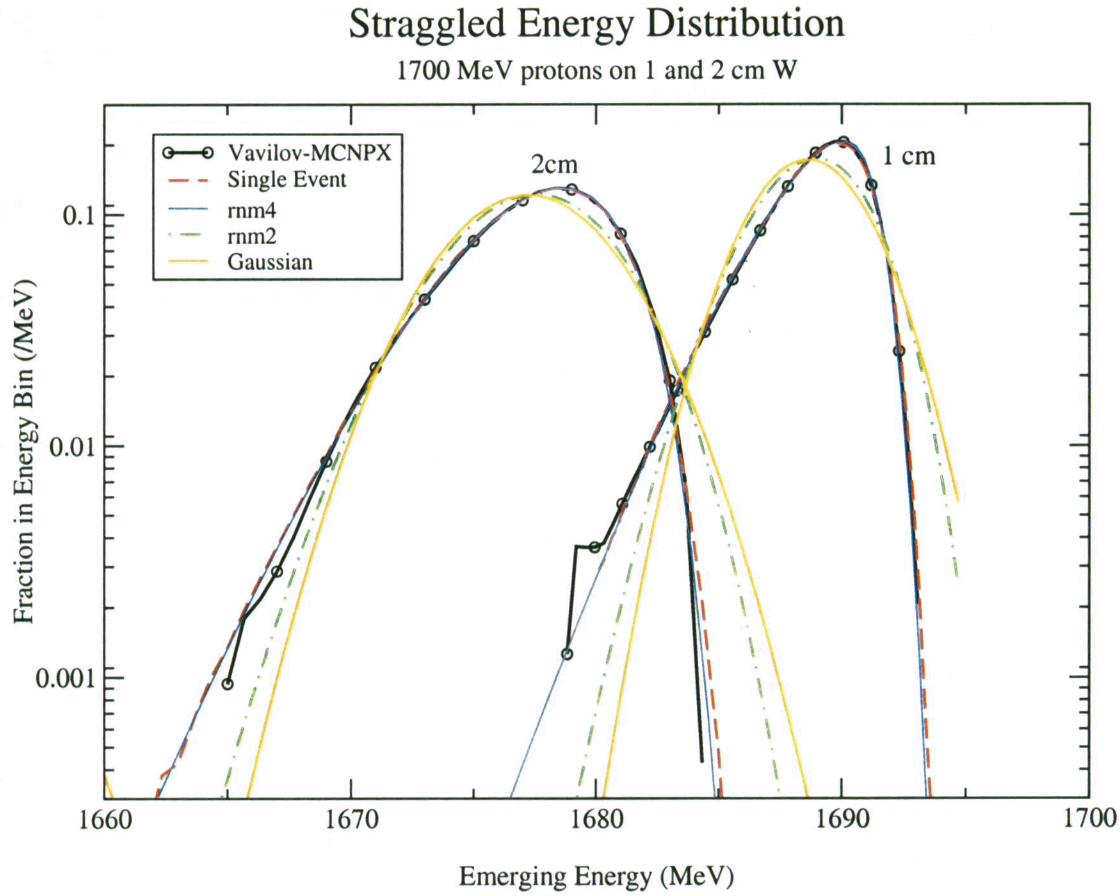
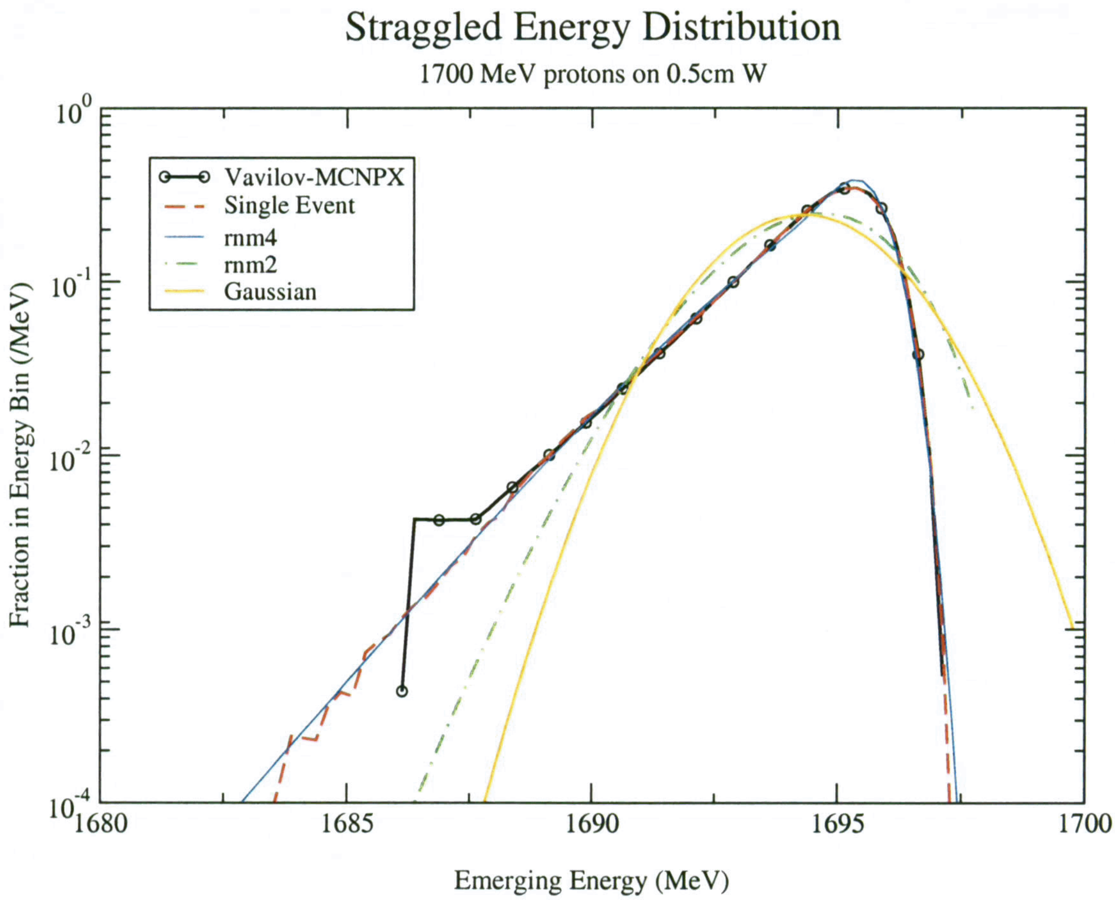
Figure Captions

Figure 1 : Straggled Proton Energy Spectra at 1 & 2cm Depth in Tungsten

Figure 2 : Straggled Proton Energy Spectrum at 0.5cm Depth in Tungsten


Straggled Energy Distribution
1700 MeV protons on 1 and 2 cm W
Vavilov-MCNPX
Single Event
rnm4
rnm2
Gaussian
2cm
1 cm
0.1
0.01
0.001
Fraction in Energy Bin (/MeV)
1660
1670
1680
1690
1700
Emerging Energy (MeV)


Straggled Energy Distribution
1700 MeV protons on 0.5cm W
Vavilov-MCNPX
Single Event
rnm4
rnm2
Gaussian
Fraction in Energy Bin (/MeV)
Emerging Energy (MeV)
10^0
10^-1
10^-2
10^-3
10^-4
1680
1685
1690
1695
1700